

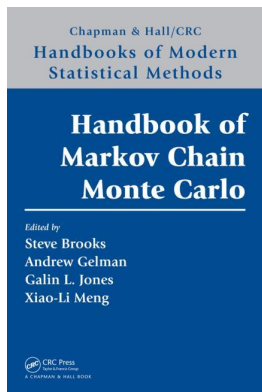
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Steve Brooks, Andrew Gelman, Galin L. Jones, Xiao-Li Meng

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Fan Yanan, Scott A. Sisson

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3

Reversible Jump MCMC

Yanan Fan and Scott A. Sisson

3.1 Introduction

The reversible jump Markov chain Monte Carlo (MCMC) sampler (Green, 1995) provides a general framework for Markov chain Monte Carlo simulation in which the dimension of the parameter space can vary between iterates of the Markov chain. The reversible jump sampler can be viewed as an extension of the Metropolis–Hastings algorithm onto more general state spaces.

To understand this in a Bayesian modeling context, suppose that for observed data \mathbf{x} we have a countable collection of candidate models $\mathcal{M} = \{\mathcal{M}_1, \mathcal{M}_2, \dots\}$ indexed by a parameter $k \in \mathcal{K}$. The index k can be considered as an auxiliary model indicator variable, such that $\mathcal{M}_{k'}$ denotes the model where $k = k'$. Each model \mathcal{M}_k has an n_k -dimensional vector of unknown parameters, $\boldsymbol{\theta}_k \in \mathbb{R}^{n_k}$, where n_k can take different values for different models $k \in \mathcal{K}$. The joint posterior distribution of $(k, \boldsymbol{\theta}_k)$ given observed data, \mathbf{x} , is obtained as the product of the likelihood, $L(\mathbf{x} | k, \boldsymbol{\theta}_k)$, and the joint prior, $p(k, \boldsymbol{\theta}_k) = p(\boldsymbol{\theta}_k | k)p(k)$, constructed from the prior distribution of $\boldsymbol{\theta}_k$ under model \mathcal{M}_k , and the prior for the model indicator k (i.e. the prior for model \mathcal{M}_k). Hence, the joint posterior is

$$\pi(k, \boldsymbol{\theta}_k | \mathbf{x}) = \frac{L(\mathbf{x} | k, \boldsymbol{\theta}_k)p(\boldsymbol{\theta}_k | k)p(k)}{\sum_{k' \in \mathcal{K}} \int_{\mathbb{R}^{n_{k'}}} L(\mathbf{x} | k', \boldsymbol{\theta}'_{k'})p(\boldsymbol{\theta}'_{k'} | k')p(k')d\boldsymbol{\theta}'_{k'}}. \quad (3.1)$$

The reversible jump algorithm uses the joint posterior distribution in Equation 3.1 as the target of an MCMC sampler over the state space $\Theta = \bigcup_{k \in \mathcal{K}} (\{k\} \times \mathbb{R}^{n_k})$, where the states of the Markov chain are of the form $(k, \boldsymbol{\theta}_k)$, the dimension of which can vary over the state space. Accordingly, from the output of a *single* Markov chain sampler, the user is able to obtain a full probabilistic description of the posterior probabilities of each model having observed the data, \mathbf{x} , in addition to the posterior distributions of the individual models.

This chapter aims to provide an overview of the reversible jump sampler. We will outline the sampler's theoretical underpinnings, present the latest and most popular techniques for enhancing algorithm performance, and discuss the analysis of sampler output. Through the use of numerous worked examples it is hoped that the reader will gain a broad appreciation of the issues involved in multi-model simulation, and the confidence to implement reversible jump samplers in the course of their own studies.

3.1.1 From Metropolis–Hastings to Reversible Jump

The standard formulation of the Metropolis–Hastings algorithm (Hastings, 1970) relies on the construction of a time-reversible Markov chain via the *detailed balance* condition. This

condition means that moves from state θ to θ' are made as often as moves from θ' to θ with respect to the target density. This is a simple way to ensure that the equilibrium distribution of the chain is the desired target distribution. The extension of the Metropolis–Hastings algorithm to the setting where the dimension of the parameter vector varies is more challenging theoretically, but the resulting algorithm is surprisingly simple to follow.

For the construction of a Markov chain on a general state space Θ with invariant or stationary distribution π , the detailed balance condition can be written as

$$\int_{(\theta, \theta') \in \mathcal{A} \times \mathcal{B}} \pi(d\theta)P(\theta, d\theta') = \int_{(\theta, \theta') \in \mathcal{A} \times \mathcal{B}} \pi(d\theta')P(\theta', d\theta) \tag{3.2}$$

for all Borel sets $\mathcal{A} \times \mathcal{B} \subset \Theta$, where P is a general Markov transition kernel (Green, 2001).

As with the standard Metropolis–Hastings algorithm, Markov chain transitions from a current state $\theta = (k, \theta'_k) \in \mathcal{A}$ in model \mathcal{M}_k are realized by first proposing a new state $\theta' = (k', \theta'_{k'}) \in \mathcal{B}$ in model $\mathcal{M}_{k'}$ from a proposal distribution $q(\theta, \theta')$. The detailed balance condition (Equation 3.2) is enforced through the acceptance probability, where the move to the candidate state θ' is accepted with probability $\alpha(\theta, \theta')$. If rejected, the chain remains at the current state θ in model \mathcal{M}_k . Under this mechanism (Green, 2001, 2003), Equation 3.2 becomes

$$\int_{(\theta, \theta') \in \mathcal{A} \times \mathcal{B}} \pi(\theta | \mathbf{x})q(\theta, \theta')\alpha(\theta, \theta')d\theta d\theta' = \int_{(\theta, \theta') \in \mathcal{A} \times \mathcal{B}} \pi(\theta' | \mathbf{x})q(\theta', \theta)\alpha(\theta', \theta)d\theta d\theta', \tag{3.3}$$

where the distributions $\pi(\theta | \mathbf{x})$ and $\pi(\theta' | \mathbf{x})$ are posterior distributions with respect to model \mathcal{M}_k and $\mathcal{M}_{k'}$, respectively.

One way to enforce Equation 3.3 is by setting the acceptance probability as

$$\alpha(\theta, \theta') = \min \left\{ 1, \frac{\pi(\theta | \mathbf{x})q(\theta, \theta')}{\pi(\theta' | \mathbf{x})q(\theta', \theta)} \right\}, \tag{3.4}$$

where $\alpha(\theta', \theta)$ is similarly defined. This resembles the usual Metropolis–Hastings acceptance ratio (Green, 1995; Tierney, 1998). It is straightforward to observe that this formulation includes the standard Metropolis–Hastings algorithm as a special case.

Accordingly, a reversible jump sampler with N iterations is commonly constructed as follows:

- Step 1. Initialize k and θ_k at iteration $t = 1$.
- Step 2. For iteration $t \geq 1$ perform
 - *Within-model move*: with a fixed model k , update the parameters θ_k according to any MCMC updating scheme.
 - *Between-models move*: simultaneously update model indicator k and the parameters θ_k according to the general reversible proposal/acceptance mechanism (Equation 3.4).
- Step 3. Increment iteration $t = t + 1$. If $t < N$, go to Step 2.

3.1.2 Application Areas

Statistical problems in which the number of unknown model parameters is itself unknown are extensive, and as such the reversible jump sampler has been implemented in analyses

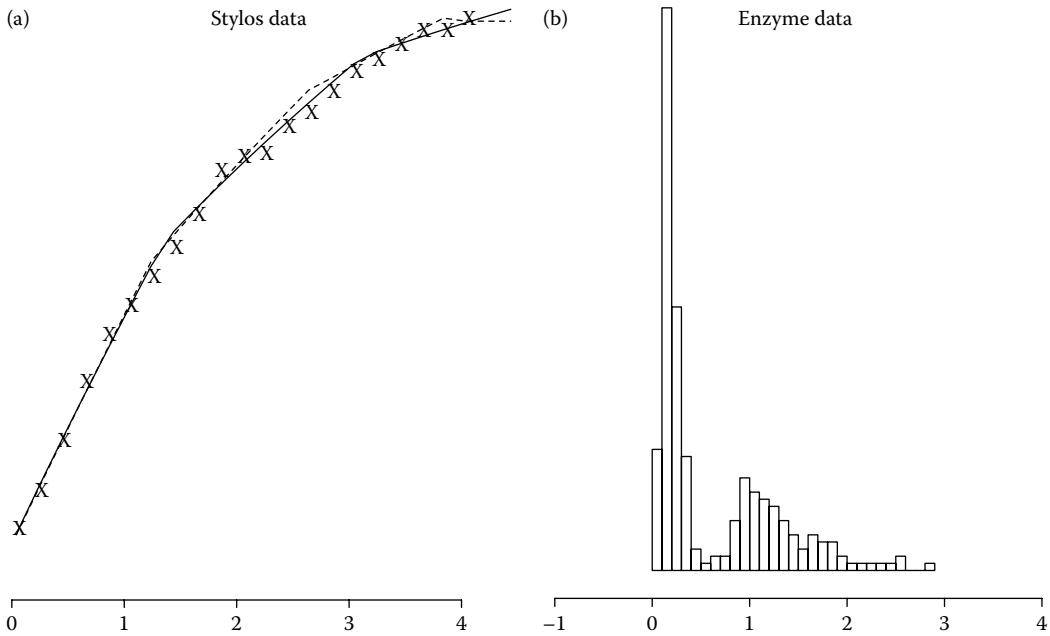


FIGURE 3.1

Examples of (a) change-point modeling and (b) mixture models. (a) With the Stylos tombs data set (crosses), a piecewise log-linear curve can be fitted between unknown change points. Illustrated are 2 (solid line) and 3 (dashed line) change points. (b) The histogram of the enzymatic activity data set suggests clear groupings of metabolizers, although the number of such groupings is not clear. (From Sisson, S. A. and Fan, Y. 2007. *Statistics and Computing*, 17:357–367. With permission.)

throughout a wide range of scientific disciplines over the last 15 years. Within the statistical literature, these predominantly concern Bayesian model determination problems (Sisson, 2005). Some of the commonly recurring models in this setting are described below.

Change-point models One of the original applications of the reversible jump sampler was in Bayesian change-point problems, where both the number and location of change points in a system is unknown *a priori*. For example, Green (1995) analyzed mining disaster count data using a Poisson process with the rate parameter described as a step function with an unknown number and location of steps. Fan and Brooks (2000) applied the reversible jump sampler to model the shape of prehistoric tombs, where the curvature of the dome changes an unknown number of times. Figure 3.1a shows the plot of depths and radii of one of the tombs from Crete in Greece. The data appear to be piecewise log-linear, with possibly two or three change points.

Finite mixture models Mixture models are commonly used where each data observation is generated according to some underlying categorical mechanism. This mechanism is typically unobserved, so there is uncertainty regarding which component of the resulting mixture distribution each data observation was generated from, in addition to uncertainty over the number of mixture components. A mixture model with k components for the observed data \mathbf{x} takes the form

$$f(\mathbf{x} | \boldsymbol{\theta}_k) = \sum_{j=1}^k w_j f_j(\mathbf{x} | \boldsymbol{\phi}_j) \tag{3.5}$$

with $\theta_k = (\phi_1, \dots, \phi_k)$, where w_j is the weight of the j th mixture component f_j , whose parameter vector is denoted by ϕ_j , and where $\sum_{j=1}^k w_j = 1$. The number of mixture components, k , is also unknown.

Figure 3.1b illustrates the distribution of enzymatic activity in the blood for 245 individuals. Richardson and Green (1997) analyzed these data using a mixture of normal densities to identify subgroups of slow or fast metabolizers. The multimodal nature of the data suggests the existence of such groups, but the number of distinct groupings is less clear. Tadesse et al. (2005) extend this normal mixture model for the purpose of clustering high-dimensional data.

Variable selection The problem of variable selection arises when modeling the relationship between a response variable, Y , and p potential explanatory variables x_1, \dots, x_p . The multi-model setting emerges when attempting to identify the most relevant subsets of predictors, making it a natural candidate for the reversible jump sampler. For example, under a regression model with normal errors we have

$$Y = X_\gamma \beta_\gamma + \epsilon \quad \text{with } \epsilon \sim N(0, \sigma^2 I), \tag{3.6}$$

where $\gamma = (\gamma_1, \dots, \gamma_p)$ is a binary vector indexing the subset of x_1, \dots, x_p to be included in the linear model, X_γ is the design matrix whose columns correspond to the indexed subset given by γ , and β_γ is the corresponding subset of regression coefficients. For examples and algorithms in this setting and beyond, see, for example, George and McCulloch (1993), Smith and Kohn (1996), and Nott and Leonte (2004).

Nonparametrics Within Bayesian nonparametrics, many authors have successfully explored the use of the reversible jump sampler as a method to automate the knot selection process when using a P th-order spline model for curve fitting (Denison et al., 1998; DiMatteo et al., 2001). Here, a curve f is estimated by

$$f(x) = \alpha_0 + \sum_{j=1}^P \alpha_j x^j + \sum_{i=1}^k \eta_i (x - \kappa_i)_+^P, \quad x \in [a, b],$$

where $z_+ = \max(0, z)$ and $\kappa_i, i = 1, \dots, k$, represent the locations of k knot points (Hastie and Tibshirani, 1990). Under this representation, fitting the curve consists of estimating the unknown number of knots k , the knot locations κ_i and the corresponding regression coefficients α_j and η_i , for $j = 0, \dots, P$ and $i = 1, \dots, k$.

Time series models In the modeling of temporally dependent data, x_1, \dots, x_T , multiple models naturally arise under uncertainty over the degree of dependence. For example, under a k th-order autoregressive process

$$X_t = \sum_{\tau=1}^k a_\tau X_{t-\tau} + \epsilon_t, \quad \text{with } t = k + 1, \dots, T, \tag{3.7}$$

where $\epsilon_t \sim WN(0, \sigma^2)$, the order, k , of the autoregression is commonly unknown, in addition to the coefficients a_τ . Brooks et al. (2003c), Ehlers and Brooks (2003), and Vermaak et al. (2004) each detail descriptions on the use of reversible jump samplers for this class of problems.

The reversible jump algorithm has had a compelling influence in the statistical and mainstream scientific research literatures. In general, the large majority of application areas have tended to be computationally or biologically related (Sisson, 2005). Accordingly a large

number of developmental and application studies can be found in the signal processing literature and the related fields of computer vision and image analysis. Epidemiological and medical studies also feature strongly.

This chapter is structured as follows: In Section 3.2 we present a detailed description of how to implement the reversible jump sampler and review methods to improve sampler performance. Section 3.3 examines post-simulation analysis, including label switching problems when identifiability is an issue, and convergence assessment. In Section 3.4 we review related sampling methods in the statistical literature, and conclude with discussion on possible future research directions for the field. Other useful reviews of reversible jump MCMC can be found in Green (2003) and Sisson (2005).

3.2 Implementation

In practice, the construction of proposal moves between different models is achieved via the concept of “dimension matching.” Most simply, under a general Bayesian model determination setting, suppose that we are currently in state (k, θ_k) in model \mathcal{M}_k , and we wish to propose a move to a state $(k', \theta'_{k'})$ in model $\mathcal{M}_{k'}$, which is of a higher dimension, so that $n_{k'} > n_k$. In order to “match dimensions” between the two model states, a random vector \mathbf{u} of length $d_{k \rightarrow k'} = n_{k'} - n_k$ is generated from a known density $q_{d_{k \rightarrow k'}}(\mathbf{u})$. The current state θ_k and the random vector \mathbf{u} are then mapped to the new state $\theta'_{k'} = g_{k \rightarrow k'}(\theta_k, \mathbf{u})$ through a one-to-one mapping function $g_{k \rightarrow k'} : \mathbb{R}^{n_k} \times \mathbb{R}^{d_k} \rightarrow \mathbb{R}^{n_{k'}}$. The acceptance probability of this proposal, combined with the joint posterior expression of Equation 3.1, becomes

$$\alpha[(k, \theta_k), (k', \theta'_{k'})] = \min \left\{ 1, \frac{\pi(k', \theta'_{k'} | \mathbf{x})q(k' \rightarrow k)}{\pi(k, \theta_k | \mathbf{x})q(k \rightarrow k')q_{d_{k \rightarrow k'}}(\mathbf{u})} \left| \frac{\partial g_{k \rightarrow k'}(\theta_k, \mathbf{u})}{\partial(\theta_k, \mathbf{u})} \right| \right\}, \quad (3.8)$$

where $q(k \rightarrow k')$ denotes the probability of proposing a move from model \mathcal{M}_k to model $\mathcal{M}_{k'}$, and the final term is the determinant of the Jacobian matrix, often referred to in the reversible jump literature simply as the Jacobian. This term arises through the change of variables via the function $g_{k \rightarrow k'}$, which is required when used with respect to the integral equation (Equation 3.3). Note that the normalization constant in Equation 3.1 is not needed to evaluate the above ratio. The reverse move proposal, from model $\mathcal{M}_{k'}$ to \mathcal{M}_k , is made deterministically in this setting, and is accepted with probability

$$\alpha[(k', \theta'_{k'}), (k, \theta_k)] = \alpha[(k, \theta_k), (k', \theta'_{k'})]^{-1}.$$

More generally, we can relax the condition on the length of the vector \mathbf{u} by allowing $d_{k \rightarrow k'} \geq n_{k'} - n_k$. In this case, nondeterministic reverse moves can be made by generating a $d_{k' \rightarrow k}$ -dimensional random vector $\mathbf{u}' \sim q_{d_{k' \rightarrow k}}(\mathbf{u}')$, such that the dimension matching condition, $n_k + d_{k \rightarrow k'} = n_{k'} + d_{k' \rightarrow k}$, is satisfied. Then a reverse mapping is given by $\theta_k = g_{k' \rightarrow k}(\theta'_{k'}, \mathbf{u}')$, such that $\theta_k = g_{k' \rightarrow k}(g_{k \rightarrow k'}(\theta_k, \mathbf{u}), \mathbf{u}')$ and $\theta'_{k'} = g_{k \rightarrow k'}(g_{k' \rightarrow k}(\theta'_{k'}, \mathbf{u}'), \mathbf{u})$. The acceptance probability corresponding to Equation 3.8 then becomes

$$\alpha[(k, \theta_k), (k', \theta'_{k'})] = \min \left\{ 1, \frac{\pi(k', \theta'_{k'} | \mathbf{x})q(k' \rightarrow k)q_{d_{k' \rightarrow k}}(\mathbf{u}')}{\pi(k, \theta_k | \mathbf{x})q(k \rightarrow k')q_{d_{k \rightarrow k'}}(\mathbf{u})} \left| \frac{\partial g_{k \rightarrow k'}(\theta_k, \mathbf{u})}{\partial(\theta_k, \mathbf{u})} \right| \right\}. \quad (3.9)$$

Example: Dimension Matching

Consider the illustrative example given in Green (1995) and Brooks (1998). Suppose that model \mathcal{M}_1 has states ($k = 1, \theta_1 \in \mathbb{R}^1$) and model \mathcal{M}_2 has states ($k = 2, \theta_2 \in \mathbb{R}^2$). Let $(1, \theta^*)$ denote the current state in \mathcal{M}_1 and $(2, (\theta^{(1)}, \theta^{(2)}))$ denote the proposed state in \mathcal{M}_2 . Under dimension matching, we might generate a random scalar u , and let $\theta^{(1)} = \theta^* + u$ and $\theta^{(2)} = \theta^* - u$, with the reverse move given deterministically by $\theta^* = \frac{1}{2} (\theta^{(1)} + \theta^{(2)})$.

Example: Moment Matching in a Finite Mixture of Univariate Normals

Under the finite mixture of univariate normals model, the observed data, \mathbf{x} , has density given by Equation 3.5, where the j th mixture component $f_j(\mathbf{x} | \phi_j) = \phi(\mathbf{x} | \mu_j, \sigma_j)$ is the $N(\mu_j, \sigma_j)$ density. For between-model moves, Richardson and Green (1997) implement a split (one component into two) and merge (two components into one) strategy which satisfies the dimension matching requirement. (See Dellaportas and Papageorgiou (2006) for an alternative approach.)

When two normal components j_1 and j_2 are merged into one, j^* , Richardson and Green (1997) propose a deterministic mapping which maintains the zeroth, first, and second moments:

$$\begin{aligned}
 w_{j^*} &= w_{j_1} + w_{j_2} \\
 w_{j^*} \mu_{j^*} &= w_{j_1} \mu_{j_1} + w_{j_2} \mu_{j_2} \\
 w_{j^*} (\mu_{j^*}^2 + \sigma_{j^*}^2) &= w_{j_1} (\mu_{j_1}^2 + \sigma_{j_1}^2) + w_{j_2} (\mu_{j_2}^2 + \sigma_{j_2}^2)
 \end{aligned}
 \tag{3.10}$$

The split move is proposed as

$$\begin{aligned}
 w_{j_1} &= w_{j^*} * u_1, & w_{j_2} &= w_{j^*} * (1 - u_1) \\
 \mu_{j_1} &= \mu_{j^*} - u_2 \sigma_{j^*} \sqrt{\frac{w_{j_2}}{w_{j_1}}} \\
 \mu_{j_2} &= \mu_{j^*} + u_2 \sigma_{j^*} \sqrt{\frac{w_{j_1}}{w_{j_2}}} \\
 \sigma_{j_1}^2 &= u_3 (1 - u_2^2) \sigma_{j^*}^2 \frac{w_{j^*}}{w_{j_1}} \\
 \sigma_{j_2}^2 &= (1 - u_3) (1 - u_2^2) \sigma_{j^*}^2 \frac{w_{j^*}}{w_{j_2}}
 \end{aligned}
 \tag{3.11}$$

where the random scalars $u_1, u_2 \sim \text{Beta}(2, 2)$ and $u_3 \sim \text{Beta}(1, 1)$. In this manner, dimension matching is satisfied, and the acceptance probability for the split move is calculated according to Equation 3.8, with the acceptance probability of the reverse merge move given by the reciprocal of this value.

3.2.1 Mapping Functions and Proposal Distributions

While the ideas behind dimension matching are conceptually simple, their implementation is complicated by the arbitrariness of the mapping function $g_{k \rightarrow k'}$ and the proposal distributions, $q_{d_{k \rightarrow k'}}(\mathbf{u})$, for the random vectors \mathbf{u} . Since mapping functions effectively express

functional relationships between the parameters of different models, good mapping functions will clearly improve sampler performance in terms of between-model acceptance rates and chain mixing. The difficulty is that even in the simpler setting of nested models, good relationships can be hard to define, and in more general settings, parameter vectors between models may not be obviously comparable.

The only additional degree of freedom to improve between-model proposals is by choosing the form and parameters of the proposal distribution $q_{d_{k \rightarrow k'}}(\mathbf{u})$. However, there are no obvious criteria to guide this choice. Contrast this to within-model, random-walk Metropolis–Hastings moves on a continuous target density, whereby proposed moves close to the current state can have an arbitrarily large acceptance probability, and proposed moves far from the current state have low acceptance probabilities. This concept of “local” moves may be partially translated on to model space ($k \in \mathcal{K}$): proposals from θ_k in model \mathcal{M}_k to $\theta_{k'}$ in model $\mathcal{M}_{k'}$ will tend to have larger acceptance probabilities if their likelihood values are similar, that is, $L(\mathbf{x} | k, \theta_k) \approx L(\mathbf{x} | k', \theta_{k'})$. For example, in the analysis of Bayesian mixture models, Richardson and Green (1997) propose “birth/death” and “split/merge” mappings of mixture components for the between-model move, while keeping other components unchanged. Hence, the proposed moves necessarily will have similar likelihood values to the current state. However, in general the notion of “local” move proposals does not easily extend to the parameter vectors of different models, unless considering simplified settings (e.g. nested models). In the general case, good mixing properties are achieved by the alignment of regions of high posterior probability between models.

Notwithstanding these difficulties, reversible jump MCMC is often associated with poor sampler performance. However, failure to realize acceptable sampler performance should only be considered a result of poorly constructed between-model mappings or inappropriate proposal distributions. It should even be anticipated that implementing a multi-model sampler may result in improved chain mixing, even when the inferential target distribution is a single model. In this case, sampling from a single model posterior with an “overly sophisticated” machinery is loosely analogous to the extra performance gained with augmented state space sampling methods. For example, in the case of a finite mixture of normal distributions, Richardson and Green (1997) report markedly superior sampler mixing when conditioning on there being exactly three mixture components, in comparison with the output generated by a fixed-dimension sampler. George et al. (1999) similarly obtain improved chain performance in a single model, by performing “birth-then-death” moves simultaneously so that the dimension of the model remains constant. Green (2003) presents a short study on which inferential circumstances determine whether the adoption of a multi-model sampler may be beneficial in this manner. Conversely, Han and Carlin (2001) provide an argument to suggest that multi-model sampling may have a detrimental effect on efficiency.

3.2.2 Marginalization and Augmentation

Depending on the aim or the complexity of a multi-model analysis, it may be that use of reversible jump MCMC would be somewhat heavy-handed, when reduced- or fixed-dimensional samplers may be substituted. In some Bayesian model selection settings, between-model moves can be greatly simplified or even avoided if one is prepared to make certain prior assumptions, such as conjugacy or objective prior specifications. In such cases, it may be possible to analytically integrate out some or all of the parameters θ_k in the posterior distribution (Equation 3.1), reducing the sampler either to fixed dimensions, for example on model space $k \in \mathcal{K}$ only, or to a lower-dimensional set of model and parameter

space (Berger and Pericchi, 2001; DiMatteo et al., 2001; George and McCulloch, 1993; Tadesse et al., 2005). In lower dimensions, the reversible jump sampler is often easier to implement, as the problems associated with mapping function specification are conceptually simpler to resolve.

Example: Marginalization in Variable Selection

In Bayesian variable selection for normal linear models (Equation 3.6), the vector $\gamma = (\gamma_1, \dots, \gamma_p)$ is treated as an auxiliary (model indicator) variable, where

$$\gamma_i = \begin{cases} 1, & \text{if predictor } x_i \text{ is included in the regression,} \\ 0, & \text{otherwise.} \end{cases}$$

Under certain prior specifications for the regression coefficients β and error variance σ^2 , the β coefficients can be analytically integrated out of the posterior. A Gibbs sampler directly on model space is then available for γ (George and McCulloch, 1993; Nott and Green, 2004; Smith and Kohn, 1996).

Example: Marginalization in Finite Mixture of Multivariate Normal Models

Within the context of clustering, the parameters of the normal components are usually not of interest. Tadesse et al. (2005) demonstrate that by choosing appropriate prior distributions, the parameters of the normal components can be analytically integrated out of the posterior. The reversible jump sampler may then run on a much reduced parameter space, which is simpler and more efficient.

In a general setting, Brooks et al. (2003c) proposed a class of models based on augmenting the state space of the target posterior with an auxiliary set of state-dependent variables, \mathbf{v}_k , so that the state space of $\pi(k, \boldsymbol{\theta}_k, \mathbf{v}_k | \mathbf{x}) = \pi(k, \boldsymbol{\theta}_k | \mathbf{x})\tau_k(\mathbf{v}_k)$ is of constant dimension for all models $\mathcal{M}_k \in \mathcal{M}$. By updating \mathbf{v}_k via a (deliberately) slowly mixing Markov chain, a temporal memory is induced that persists in the \mathbf{v}_k from state to state. In this manner, the motivation behind the auxiliary variables is to improve between-model proposals, in that some memory of previous model states is retained. Brooks et al. (2003c) demonstrate that this approach can significantly enhance mixing compared to an unassisted reversible jump sampler. Although the fixed dimensionality of $(k, \boldsymbol{\theta}_k, \mathbf{v}_k)$ is later relaxed, there is an obvious analogue with product space sampling frameworks (Carlin and Chib, 1995; Godsill, 2001); see Section 3.4.2.

An alternative augmented state space modification of standard MCMC is given by Liu et al. (2001). The dynamic weighting algorithm augments the original state space by a weighting factor, which permits the Markov chain to make large transitions not allowable by the standard transition rules, subject to the computation of the correct weighting factor. Inference is then made by using the weights to compute importance sampling estimates rather than simple Monte Carlo estimates. This method can be used within the reversible jump algorithm to facilitate cross-model jumps.

3.2.3 Centering and Order Methods

Brooks et al. (2003c) introduce a class of methods to achieve the automatic scaling of the proposal density, $q_{d_{k \rightarrow k'}}(\mathbf{u})$, based on “local” move proposal distributions, which are centered around the point of equal likelihood values under current and proposed models. Under this scheme, it is assumed that local mapping functions $g_{k \rightarrow k'}$ are known. For a proposed move from $(k, \boldsymbol{\theta}_k)$ in \mathcal{M}_k to model $\mathcal{M}_{k'}$, the random vector “centering point”

$c_{k \rightarrow k'}(\boldsymbol{\theta}_k) = g_{k \rightarrow k'}(\boldsymbol{\theta}_k, \mathbf{u})$ is defined such that, for some particular choice of proposal vector \mathbf{u} , the current and proposed states are identical in terms of likelihood contribution, that is, $L(\mathbf{x} | k, \boldsymbol{\theta}_k) = L(\mathbf{x} | k', c_{k \rightarrow k'}(\boldsymbol{\theta}_k))$. For example, if \mathcal{M}_k is an autoregressive model of order k (Equation 3.7) and $\mathcal{M}_{k'}$ is an autoregressive model of order $k' = k + 1$, and if $c_{k \rightarrow k'}(\boldsymbol{\theta}_k) = g_{k \rightarrow k'}(\boldsymbol{\theta}_k, u) = (\boldsymbol{\theta}_k, u)$ (e.g. a local “birth” proposal), then we have $u = 0$ and $c_{k \rightarrow k'} = (\boldsymbol{\theta}_k, 0)$, as $L(\mathbf{x} | k, \boldsymbol{\theta}_k) = L(\mathbf{x} | k', (\boldsymbol{\theta}_k, 0))$.

Given the centering constraint on \mathbf{u} , if the scaling parameter in the proposal $q_{d_{k \rightarrow k'}}(\mathbf{u})$ is a scalar, then the zeroth-order method (Brooks et al., 2003c) proposes to choose this scaling parameter such that the acceptance probability $\alpha[(k, \boldsymbol{\theta}_k), (k', c_{k \rightarrow k'}(\boldsymbol{\theta}_k))]$ of a move to the centering point $c_{k \rightarrow k'}(\boldsymbol{\theta}_k)$ in model $\mathcal{M}_{k'}$ is exactly one. The argument is then that move proposals close to $c_{k \rightarrow k'}(\boldsymbol{\theta}_k)$ will also have a large acceptance probability.

For proposal distributions, $q_{d_{k \rightarrow k'}}(\mathbf{u})$, with additional degrees of freedom, a similar method based on a series of n th-order conditions (for $n \geq 1$) requires that, for the proposed move, the n th derivative (with respect to \mathbf{u}) of the acceptance probability equals the zero vector at the centering point $c_{k \rightarrow k'}(\boldsymbol{\theta}_k)$:

$$\nabla^n \alpha[(k, \boldsymbol{\theta}_k), (k', c_{k \rightarrow k'}(\boldsymbol{\theta}_k))] = \mathbf{0}. \tag{3.12}$$

That is, the m unknown parameters in the proposal distribution $q_{d_{k \rightarrow k'}}(\mathbf{u})$ are determined by solving the m simultaneous equations given by Equation 3.12 with $n = 1, \dots, m$. The idea behind the n th-order method is that the concept of closeness to the centering point under the zeroth-order method is relaxed. By enforcing zero derivatives of $\alpha[(k, \boldsymbol{\theta}_k), (k', c_{k \rightarrow k'}(\boldsymbol{\theta}_k))]$, the acceptance probability will become flatter around $c_{k \rightarrow k'}(\boldsymbol{\theta}_k)$. Accordingly this allows proposals further away from the centering point to still be accepted with a reasonably high probability. This will ultimately induce improved chain mixing.

With these methods, proposal distribution parameters are adapted to the current state of the chain, $(k, \boldsymbol{\theta}_k)$, rather than relying on a constant proposal parameter vector for all state transitions. It can be shown that for a simple two-model case, the n th-order conditions are optimal in terms of the capacitance of the algorithm (Lawler and Sokal, 1988). See also Ehlers and Brooks (2003) for an extension to a more general setting, and Ntzoufras et al. (2003) for a centering method in the context of linear models.

One caveat with the centering schemes is that they require specification of the between-model mapping function $g_{k \rightarrow k'}$, although these methods compensate for poor choices of mapping functions by selecting the best set of parameters for the given mapping. Recently, Ehlers and Brooks (2008) suggest the posterior conditional distribution $\pi(k', \mathbf{u} | \boldsymbol{\theta}_k)$ as the proposal for the random vector \mathbf{u} , side-stepping the need to construct a mapping function. In this case, the full conditionals either must be known or need to be approximated.

Example: The Zeroth-Order Method for an Autoregressive Model

Brooks et al. (2003c) consider the AR model with unknown order k (Equation 3.7), assuming Gaussian noise $\epsilon_t \sim N(0, \sigma_\epsilon^2)$ and a uniform prior on k , where $k = 1, 2, \dots, k_{\max}$. Within each model \mathcal{M}_k , independent $N(0, \sigma_a^2)$ priors are adopted for the AR coefficients $a_\tau, \tau = 1, \dots, k$, with an inverse gamma prior for σ_ϵ^2 . Suppose moves are made from model \mathcal{M}_k to model $\mathcal{M}_{k'}$ such that $k' = k + 1$. The move from $\boldsymbol{\theta}_k$ to $\boldsymbol{\theta}_{k'}$ is achieved by generating a random scalar $u \sim q(u) = N(0, 1)$, and defining the mapping function as $\boldsymbol{\theta}'_{k'} = g_{k \rightarrow k'}(\boldsymbol{\theta}_k, u) = (\boldsymbol{\theta}_k, \sigma u)$. The centering point $c_{k \rightarrow k'}(\boldsymbol{\theta}_k)$ then occurs at the point $u = 0$, or $\boldsymbol{\theta}'_{k'} = (\boldsymbol{\theta}_k, 0)$.

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Under the mapping $g_{k \rightarrow k'}$, the Jacobian is σ , and the acceptance probability (Equation 3.8) for the move from $(k, \boldsymbol{\theta}_k)$ to $(k', c_{k \rightarrow k'}(\boldsymbol{\theta}_k))$ is given by $\alpha[(k, \boldsymbol{\theta}_k), (k', (\boldsymbol{\theta}_k, 0))] = \min(1, A)$ where

$$A = \frac{\pi(k', (\boldsymbol{\theta}_k, 0) | \mathbf{x})q(k' \rightarrow k)\sigma}{\pi(k, \boldsymbol{\theta}_k | \mathbf{x})q(k \rightarrow k')q(0)} = \frac{(2\pi\sigma_a^2)^{-1/2} q(k' \rightarrow k)\sigma}{q(k \rightarrow k')(2\pi)^{-1/2}}.$$

Note that since the likelihoods are equal at the centering point, and the priors common to both models cancel in the posterior ratio, A is only a function of the prior density for the parameter a_{k+1} evaluated at 0, the proposal distributions and the Jacobian. Hence, we solve $A = 1$ to obtain

$$\sigma^2 = \sigma_a^2 \left(\frac{q(k \rightarrow k')}{q(k' \rightarrow k)} \right)^2.$$

Thus in this case, the proposal variance is not dependent on the model parameter $(\boldsymbol{\theta}_k)$ or data (\mathbf{x}) . It depends only on the prior variance, σ_a , and the model states, k, k' .

Example: The Second-Order Method for Moment Matching

Consider the moment matching in a finite mixture of univariate normals example of Section 3.2. The mapping functions $g_{k' \rightarrow k}$ and $g_{k \rightarrow k'}$ are respectively given by Equations 3.10 and 3.11, with the random numbers u_1, u_2, u_3 drawn from independent beta distributions with unknown parameter values, so that $q_{p_i, q_i}(u_i): u_i \sim \text{Beta}(p_i, q_i), i = 1, 2, 3$.

Consider the split move, Equation 3.11. To apply the second-order method of Brooks et al. (2003c), we first locate a centering point, $c_{k \rightarrow k'}(\boldsymbol{\theta}_k)$, achieved by setting $u_1 = 1, u_2 = 0$, and $u_3 \equiv u_1 = 1$ by inspection. Hence, at the centering point, the two new (split) components j_1 and j_2 will have the same location and scale as the j^* component, with new weights $w_{j_1} = w_{j^*}$ and $w_{j_2} = 0$ and all observations allocated to component j_1 . Accordingly this will produce identical likelihood contributions. Note that to obtain equal variances for the split proposal, substitute the expressions for w_{j_1} and w_{j_2} into those for $\sigma_{j_1}^2 = \sigma_{j_2}^2$.

Following Richardson and Green (1997), the acceptance probability of the split move evaluated at the centering point is then proportional (with respect to \mathbf{u}) to

$$\begin{aligned} & \log A[(k, \boldsymbol{\theta}_k), (k', c_{k \rightarrow k'}(\boldsymbol{\theta}_k))] \\ & \propto l_{j_1} \log(w_{j_1}) + l_{j_2} \log(w_{j_2}) - \frac{l_{j_1}}{2} \log(\sigma_{j_1}^2) - \frac{l_{j_2}}{2} \log(\sigma_{j_2}^2) - \frac{1}{2\sigma_{j_1}^2} \sum_{l=1}^{l_{j_1}} (y_l - \mu_{j_1})^2 \\ & \quad - \frac{1}{2\sigma_{j_2}^2} \sum_{l=1}^{l_{j_2}} (y_l - \mu_{j_2})^2 + (\delta - 1 + l_{j_1}) \log(w_{j_1}) + (\delta - 1 + l_{j_2}) \log(w_{j_2}) \\ & \quad - \left\{ \frac{1}{2} \kappa [(\mu_{j_1} - \xi)^2 + (\mu_{j_2} - \xi)^2] \right\} - (\alpha + 1) \log(\sigma_{j_1}^2 \sigma_{j_2}^2) - \beta (\sigma_{j_1}^{-2} + \sigma_{j_2}^{-2}) \\ & \quad - \log[q_{p_1, q_1}(u_1)] - \log[q_{p_2, q_2}(u_2)] - \log[q_{p_3, q_3}(u_3)] + \log(|\mu_{j_1} - \mu_{j_2}|) \\ & \quad + \log(\sigma_{j_1}^2) + \log(\sigma_{j_2}^2) - \log(u_2) - \log(1 - u_2^2) - \log(u_3) - \log(1 - u_3), \end{aligned} \quad (3.13)$$

where l_{j_1} and l_{j_2} respectively denote the number of observations allocated to components j_1 and j_2 , and where $\delta, \alpha, \beta, \xi$ and κ are hyperparameters as defined by Richardson and Green (1997).

Thus, for example, to obtain the proposal parameter values p_1 and q_1 for u_1 , we solve the first- and second-order derivatives of the acceptance probability (Equation 3.13) with respect to u_1 . This yields

$$\frac{\partial \log \alpha [(k, \boldsymbol{\theta}_k), (k', c_{k \rightarrow k'}(\boldsymbol{\theta}_k))]}{\partial u_1} = \frac{\delta + 2l_{j_1} - p_1}{u_1} + \frac{q_1 - \delta - 2l_{j_2}}{(1 - u_1)}$$

$$\frac{\partial^2 \log \alpha [(k, \boldsymbol{\theta}_k), (k', c_{k \rightarrow k'}(\boldsymbol{\theta}_k))]}{\partial u_1^2} = -\frac{\delta + 2l_{j_1} - p_1}{u_1^2} + \frac{q_1 - \delta - 2l_{j_2}}{(1 - u_1)^2}.$$

Equating these to zero and solving for p_1 and q_1 at the centering points (with $l_{j_1} = l_{j^*}$ and $l_{j_2} = 0$) gives $p_1 = \delta + 2l_{j^*}$ and $q_1 = \delta$. Thus the parameter p_1 depends on the number of observations allocated to the component being split. Similar calculations to the above give solutions for $p_2, q_2, p_3,$ and q_3 .

3.2.4 Multi-Step Proposals

Green and Mira (2001) introduce a procedure for learning from rejected between-model proposals based on an extension of the splitting rejection idea of Tierney and Mira (1999). After rejecting a between-model proposal, the procedure makes a second proposal, usually under a modified proposal mechanism, and potentially dependent on the value of the rejected proposal. In this manner, a limited form of adaptive behavior may be incorporated into the proposals. The procedure is implemented via a modified Metropolis–Hastings acceptance probability, and may be extended to more than one sequential rejection (Trias et al., 2009). Delayed-rejection schemes can reduce the asymptotic variance of ergodic averages by reducing the probability of the chain remaining in the same state (Peskun, 1973; Tierney, 1998), however there is an obvious tradeoff with the extra move construction and computation required.

For clarity of exposition, in the remainder of this section we denote the current state of the Markov chain in model \mathcal{M}_k by $\mathbf{x} = (k, \boldsymbol{\theta}_k)$, and the first and second stage proposed states in model $\mathcal{M}_{k'}$ by \mathbf{y} and \mathbf{z} . Let $\mathbf{y} = g_{k \rightarrow k'}^{(1)}(\mathbf{x}, \mathbf{u}_1)$ and $\mathbf{z} = g_{k \rightarrow k'}^{(2)}(\mathbf{x}, \mathbf{u}_1, \mathbf{u}_2)$ be the mappings of the current state and random vectors $\mathbf{u}_1 \sim q_{d_{k \rightarrow k'}}^{(1)}(\mathbf{u}_1)$ and $\mathbf{u}_2 \sim q_{d_{k \rightarrow k'}}^{(2)}(\mathbf{u}_2)$ into the proposed new states. For simplicity, we again consider the framework where the dimension of model \mathcal{M}_k is smaller than that of model $\mathcal{M}_{k'}$ (i.e. $n_{k'} > n_k$) and where the reverse move proposals are deterministic. The proposal from \mathbf{x} to \mathbf{y} is accepted with the usual acceptance probability

$$\alpha_1(\mathbf{x}, \mathbf{y}) = \min \left\{ 1, \frac{\pi(\mathbf{y})q(k' \rightarrow k)}{\pi(\mathbf{x})q(k \rightarrow k')q_{d_{k \rightarrow k'}}^{(1)}(\mathbf{u}_1)} \left| \frac{\partial g_{k \rightarrow k'}^{(1)}(\mathbf{x}, \mathbf{u}_1)}{\partial(\mathbf{x}, \mathbf{u}_1)} \right| \right\}.$$

If \mathbf{y} is rejected, detailed balance for the move from \mathbf{x} to \mathbf{z} is preserved with the acceptance probability

$$\alpha_2(\mathbf{x}, \mathbf{z}) = \min \left\{ 1, \frac{\pi(\mathbf{z})q(k' \rightarrow k)[1 - \alpha_1(\mathbf{y}^*, \mathbf{z})]^{-1}}{\pi(\mathbf{x})q(k \rightarrow k')q_{d_{k \rightarrow k'}}^{(1)}(\mathbf{u}_1)q_{d_{k \rightarrow k'}}^{(2)}(\mathbf{u}_2)[1 - \alpha_1(\mathbf{x}, \mathbf{y})]} \left| \frac{\partial g_{k \rightarrow k'}^{(2)}(\mathbf{x}, \mathbf{u}_1, \mathbf{u}_2)}{\partial(\mathbf{x}, \mathbf{u}_1, \mathbf{u}_2)} \right| \right\},$$

where $\mathbf{y}^* = g_{k \rightarrow k'}^{(1)}(\mathbf{z}, \mathbf{u}_1)$. Note that the second stage proposal $\mathbf{z} = g_{k \rightarrow k'}^{(2)}(\mathbf{x}, \mathbf{u}_1, \mathbf{u}_2)$ is permitted to depend on the rejected first stage proposal \mathbf{y} (a function of \mathbf{x} and \mathbf{u}_1).

In a similar vein, Al-Awadhi et al. (2004) also acknowledged that an initial between-model proposal $\mathbf{x}' = g_{k \rightarrow k'}(\mathbf{x}, \mathbf{u})$ may be poor, and seek to adjust the state \mathbf{x}' to a region of higher posterior probability before taking the decision to accept or reject the proposal. Specifically, Al-Awadhi et al. (2004) propose to initially evaluate the proposed move to \mathbf{x}' in model $\mathcal{M}_{k'}$ through a density $\pi^*(\mathbf{x}')$ rather than the usual $\pi(\mathbf{x}')$. The authors suggest taking π^* to be some tempered distribution $\pi^* = \pi^\gamma$, $\gamma > 1$, such that the modes of π^* and π are aligned.

The algorithm then implements $\kappa \geq 1$ fixed-dimension MCMC updates, generating states $\mathbf{x}' \rightarrow \mathbf{x}^1 \rightarrow \dots \rightarrow \mathbf{x}^\kappa = \mathbf{x}^*$, with each step satisfying detailed balance with respect to π^* . This provides an opportunity for \mathbf{x}^* to move closer to the mode of π^* (and therefore π) than \mathbf{x}' . The move from \mathbf{x} in model \mathcal{M}_k to the final state \mathbf{x}^* in model $\mathcal{M}_{k'}$ (with density $\pi(\mathbf{x}^*)$) is finally accepted with probability

$$\alpha(\mathbf{x}, \mathbf{x}^*) = \min \left\{ 1, \frac{\pi(\mathbf{x}^*)\pi^*(\mathbf{x}')q(k' \rightarrow k)}{\pi(\mathbf{x})\pi^*(\mathbf{x}^*)q(k \rightarrow k')q_{d_{k \rightarrow k'}}(\mathbf{u})} \left| \frac{\partial g_{k \rightarrow k'}(\mathbf{x}, \mathbf{u})}{\partial(\mathbf{x}, \mathbf{u})} \right| \right\}.$$

The implied reverse move from model $\mathcal{M}_{k'}$ to model \mathcal{M}_k is conducted by taking the κ moves with respect to π^* first, followed by the dimension-changing move.

Various extensions can easily be incorporated into this framework, such as using a sequence of π^* distributions, resulting in a slightly modified acceptance probability expression. For instance, the standard simulated annealing framework, Kirkpatrick (1984), provides an example of a sequence of distributions which encourage moves toward posterior mode. Clearly the choice of the distribution π^* can be crucial to the success of this strategy. As with all multi-step proposals, increased computational overheads are traded for potentially enhanced between-model mixing.

3.2.5 Generic Samplers

The problem of efficiently constructing between-model mapping templates, $g_{k \rightarrow k'}$, with associated random vector proposal densities, $q_{d_{k \rightarrow k'}}$, may be approached from an alternative perspective. Rather than relying on a user-specified mapping, one strategy would be to move toward a more generic proposal mechanism altogether. A clear benefit of generic between-model moves is that they may be equally be implemented for nonnested models. While the ideal of “black-box” between-model proposals is attractive, they currently remain on the research horizon. However, a number of automatic reversible jump MCMC samplers have been proposed.

Green (2003) proposed a reversible jump analogy of the random-walk Metropolis sampler of Roberts (2003). Suppose that estimates of the first- and second-order moments of θ_k are available, for each of a small number of models, $k \in \mathcal{K}$, denoted by μ_k and $\mathbf{B}_k \mathbf{B}_k^\top$ respectively, where \mathbf{B}_k is an $n_k \times n_k$ matrix. In proposing a move from (k, θ_k) to model $\mathcal{M}_{k'}$, a new parameter vector is proposed by

$$\theta'_{k'} = \begin{cases} \mu_{k'} + \mathbf{B}_{k'} \left[\mathbf{R} \mathbf{B}_k^{-1} (\theta_k - \mu_k) \right]_1^{n_{k'}}, & \text{if } n_{k'} < n_k, \\ \mu_{k'} + \mathbf{B}_{k'} \mathbf{R} \mathbf{B}_k^{-1} (\theta_k - \mu_k), & \text{if } n_{k'} = n_k, \\ \mu_{k'} + \mathbf{B}_{k'} \mathbf{R} \left(\mathbf{B}_k^{-1} (\theta_k - \mu_k) \right)_\mathbf{u}, & \text{if } n_{k'} > n_k, \end{cases}$$

where $[\cdot]_1^m$ denotes the first m components of a vector, \mathbf{R} is a orthogonal matrix of order $\max\{n_k, n_{k'}\}$, and $\mathbf{u} \sim q_{n_{k'} - n_k}(\mathbf{u})$ is an $(n_{k'} - n_k)$ -dimensional random vector (only utilized

if $n_{k'} > n_k$, or when calculating the acceptance probability of the reverse move from model $\mathcal{M}_{k'}$ to model \mathcal{M}_k if $n_{k'} < n_k$). If $n_{k'} \leq n_k$, then the proposal $\theta'_{k'}$ is deterministic and the Jacobian is trivially calculated. Hence, the acceptance probability is given by

$$\alpha[(k, \theta_k), (k', \theta'_{k'})] = \frac{\pi(k', \theta'_{k'} | \mathbf{x}) q(k' \rightarrow k) |\mathbf{B}_{k'}|}{\pi(k, \theta_k | \mathbf{x}) q(k \rightarrow k') |\mathbf{B}_k|} \times \begin{cases} q_{n_{k'}-n_k}(\mathbf{u}), & \text{for } n_{k'} < n_k, \\ 1, & \text{for } n_{k'} = n_k, \\ \frac{1}{q_{n_k-n_{k'}}}(\mathbf{u}), & \text{for } n_{k'} > n_k. \end{cases}$$

Accordingly, if the model-specific densities $\pi(k, \theta_k | \mathbf{x})$ are unimodal with first- and second-order moments given by μ_k and $\mathbf{B}_k \mathbf{B}_k^\top$, then high between-model acceptance probabilities may be achieved. (Unitary acceptance probabilities are available if the $\pi(k, \theta_k | \mathbf{x})$ are exactly Gaussian.) Green (2003), Godsill (2003), and Hastie (2004) discuss a number of modifications to this general framework, including improving efficiency and relaxing the requirement of unimodal densities $\pi(k, \theta_k | \mathbf{x})$ to realize high between-model acceptance rates. Naturally, the required knowledge of first- and second-order moments of each model density will restrict the applicability of these approaches to moderate numbers of candidate models if these require estimation (e.g. via pilot chains).

With a similar motivation to the above, Papathomas et al. (2009) put forward the multivariate normal as proposal distribution for $\theta'_{k'}$ in the context of linear regression models, so that $\theta'_{k'} \sim N(\mu_{k'|\theta_k}, \Sigma_{k'|\theta_k})$. The authors derive estimates for the mean $\mu_{k'|\theta_k}$ and covariance $\Sigma_{k'|\theta_k}$ such that the proposed values for $\theta'_{k'}$ will on average produce conditional posterior values under model $\mathcal{M}_{k'}$ similar to those produced by the vector θ_k under model \mathcal{M}_k . In particular, consider the normal linear model in Equation 3.6, rewriting the error covariance as V , assuming equality under the two models such that $V_k = V_{k'} = V$. The parameters of the proposal distribution for $\theta'_{k'}$ are then given by

$$\begin{aligned} \mu_{k'|\theta_k} &= (X_{\gamma'}^\top V^{-1} X_{\gamma'})^{-1} X_{\gamma'}^\top V^{-1} \left\{ \gamma + B^{-1} V^{-1/2} (X_\gamma \theta_k - P_k \gamma) \right\}, \\ \Sigma_{k'|\theta_k} &= Q_{k',k'} - Q_{k',k'} Q_{k',k}^{-1} Q_{k,k} Q_{k,k'}^{-1} Q_{k,k'} + c I_{n_{k'}}, \end{aligned}$$

where γ and γ' are indicators corresponding to models \mathcal{M}_k and $\mathcal{M}_{k'}$, $B = (V + X_{\gamma'} \Sigma_{k'|\theta_k} X_{\gamma'}^\top)^{-1/2}$, $P_k = X_{\gamma'} (X_{\gamma'}^\top V^{-1} X_{\gamma'})^{-1} X_{\gamma'}^\top V^{-1}$, $Q_{k,k'} = (X_{\gamma'}^\top V^{-1} X_{\gamma'})^{-1}$, I_n is the $n \times n$ identity matrix and $c > 0$. Intuitively, the mean of this proposal distribution may be interpreted as the maximum likelihood estimate of $\theta'_{k'}$ for model $\mathcal{M}_{k'}$, plus a correction term based on the distance of the current chain state θ_k to the mode of the posterior density in model \mathcal{M}_k . The mapping between $\theta'_{k'}$ and θ_k and the random number \mathbf{u} is given by

$$\theta'_{k'} = \mu_{k'|\theta_k} + \Sigma_{k'|\theta_k}^{1/2} \mathbf{u},$$

where $\mathbf{u} \sim N(0, I_{n_{k'}})$. Accordingly the Jacobian corresponding to Equation 3.9 is given by $\left| \Sigma_{k'|\theta_k}^{1/2} \right| \left| \Sigma_{k|\theta_{k'}}^{1/2} \right|$. Under this construction, the value $c > 0$ is treated as a tuning parameter for the calibration of the acceptance probability. Quite clearly, the parameters of the between-model proposal do not require *a priori* estimation, and they adapt to the current state of the chain. The authors note that in some instances, this method produces similar results in terms of efficiency to Green (2003). One caveat is that the calculations at each proposal stage involve several inversions of matrices which can be computationally costly when the dimension is large. In addition, the method is theoretically justified for normal linear

models, but can be applied to nonnormal models when transformation of data to normality is available, as demonstrated in Papathomas et al. (2009).

Fan et al. (2009) propose to construct between-model proposals based on estimating conditional marginal densities. Suppose that it is reasonable to assume some structural similarities between the parameters θ_k and $\theta'_{k'}$ of models \mathcal{M}_k and $\mathcal{M}_{k'}$, respectively. Let c indicate the subset of the vectors $\theta_k = (\theta_k^c, \theta_k^{-c})$ and $\theta'_{k'} = (\theta'_{k'}{}^c, \theta'_{k'}{}^{-c})$ which can be kept constant between models, so that $\theta'_{k'}{}^c = \theta_k^c$. The remaining r -dimensional vector $\theta'_{k'}{}^{-c}$ is then sampled from an estimate of the factorization of the conditional posterior of $\theta'_{k'}{}^{-c} = (\theta'_{k'}{}^{-c,1}, \dots, \theta'_{k'}{}^{-c,r})$ under model $\mathcal{M}_{k'}$:

$$\pi(\theta'_{k'}{}^{-c} \mid \theta'_{k'}{}^c, \mathbf{x}) \approx \hat{\pi}_1(\theta'_{k'}{}^{-c,1} \mid \theta'_{k'}{}^c, \dots, \theta'_{k'}{}^{-c,r}, \theta'_{k'}{}^c, \mathbf{x}) \dots \hat{\pi}_{r-1}(\theta'_{k'}{}^{-c,r-1} \mid \theta'_{k'}{}^c, \theta'_{k'}{}^{-c,1}, \dots, \theta'_{k'}{}^{-c,r-2}, \theta'_{k'}{}^c, \mathbf{x}) \hat{\pi}_r(\theta'_{k'}{}^{-c,r} \mid \theta'_{k'}{}^c, \mathbf{x}).$$

The proposal $\theta'_{k'}{}^{-c}$ is drawn by first estimating $\hat{\pi}_r(\theta'_{k'}{}^{-c,r} \mid \theta'_{k'}{}^c, \mathbf{x})$ and sampling $\theta'_{k'}{}^{-c,r}$, and by then estimating $\hat{\pi}_{r-1}(\theta'_{k'}{}^{-c,r-1} \mid \theta'_{k'}{}^c, \theta'_{k'}{}^{-c,r}, \mathbf{x})$ and sampling $\theta'_{k'}{}^{-c,r-1}$, conditioning on the previously sampled point, $\theta'_{k'}{}^{-c,r}$, and so on. Fan et al. (2009) construct the conditional marginal densities by using partial derivatives of the joint density, $\pi(k', \theta'_{k'} \mid \mathbf{x})$, to provide gradient information within a marginal density estimator. As the conditional marginal density estimators are constructed using a combination of samples from the prior distribution and gridded values, they can be computationally expensive to construct, particularly if high-dimensional moves are attempted, for example $\theta'_{k'}{}^{-c} = \theta'_{k'}$. However, this approach can be efficient, and also adapts to the current state of the sampler.

3.3 Post Simulation

3.3.1 Label Switching

The so-called “label switching” problem occurs when the posterior distribution is invariant under permutations in the labeling of the parameters. This results in the parameters having identical marginal posterior distributions. For example, in the context of a finite mixture model (Equation 3.5), the parameters of each mixture component, ϕ_j , are unidentifiable under a symmetric prior. This causes problems in the interpretation of the MCMC output. While this problem is general, in that it is not restricted to the multi-model case, as many applications of the reversible jump sampler encounter this type of problem, we discuss some methods of overcoming this issue below.

The conceptually simplest method of circumventing nonidentifiability is to impose artificial constraints on the parameters. For example, if μ_j denotes the mean of the j th Gaussian mixture component, then one such constraint could be $\mu_1 < \dots < \mu_k$ (Richardson and Green, 1997). However, the effectiveness of this approach is not always guaranteed (Jasra et al., 2005). One of the main problems with such constraints is that they are often artificial, being imposed for inferential convenience rather than as a result of genuine knowledge about the model. Furthermore, suitable constraints can be difficult or almost impossible to find (Frühwirth-Schnatter, 2001).

Alternative approaches to handling nonidentifiability involve the post-processing of MCMC output. Stephens (2000b) gives an inferential method based on the relabeling of components with respect to the permutation which minimizes the posterior expected loss. Celeux et al. (2000), Hurn et al. (2003), and Sisson and Hurn (2004) adopt a fully decision-theoretic approach, where for every posterior quantity of interest, an appropriate (possibly

multi-model) loss function is constructed and minimized. Each of these methods can be computationally expensive.

3.3.2 Convergence Assessment

Under the assumption that an acceptably efficient method of constructing a reversible jump sampler is available, one obvious pre-requisite to inference is that the Markov chain converges to its equilibrium state. Even in fixed dimension problems, theoretical convergence bounds are in general difficult or impossible to determine. In the absence of such theoretical results, convergence diagnostics based on empirical statistics computed from the sample path of multiple chains are often the only available tool. An obvious drawback of the empirical approach is that such diagnostics invariably fail to detect a lack of convergence when parts of the target distribution are missed entirely by all replicate chains. Accordingly, these are necessary rather than sufficient indicators of chain convergence; see Mengersen et al. (1999) and Cowles and Carlin (1996) for comparative reviews under fixed dimension MCMC.

The reversible jump sampler generates additional problems in the design of suitable empirical diagnostics, since most of these depend on the identification of suitable scalar statistics of the parameters' sample paths. However, in the multi-model case, these parameters may no longer retain the same interpretation. In addition, convergence is required not only within each of a potentially large number of models, but also across models with respect to posterior model probabilities.

One obvious approach would be the implementation of independent sub-chain assessments, both within models and for the model indicator $k \in \mathcal{K}$. With focus purely on model selection, Brooks et al. (2003b) propose various diagnostics based on the sample path of the model indicator, k , including nonparametric hypothesis tests such as the χ^2 and Kolmogorov–Smirnov tests. In this manner, distributional assumptions of the models (but not the statistics) are circumvented at the price of associating marginal convergence of k with convergence of the full posterior density.

Brooks and Giudici (2000) propose the monitoring of functionals of parameters which retain their interpretations as the sampler moves between models. The deviance is suggested as a default choice in the absence of superior alternatives. A two-way ANOVA decomposition of the variance of such a functional is formed over multiple chain replications, from which the potential scale reduction factor (PSRF) (Gelman and Rubin, 1992) can be constructed and monitored. Castelloe and Zimmerman (2002) extend this approach firstly to an unbalanced (weighted) two-way ANOVA, to prevent the PRSF being dominated by a few visits to rare models, with the weights being specified in proportion to the frequency of model visits. Castelloe and Zimmerman (2002) also extend their diagnostic to the multivariate (MANOVA) setting on the observation that monitoring several functionals of marginal parameter subsets is more robust than monitoring a single statistic. This general method is clearly reliant on the identification of useful statistics to monitor, but is also sensitive to the extent of approximation induced by violations of the ANOVA assumptions of independence and normality.

Sisson and Fan (2007) propose diagnostics when the underlying model can be formulated in the marked point process framework (Diggle, 1983; Stephens, 2000a). For example, a mixture of an unknown number of univariate normal densities (Equation 3.5) can be represented as a set of k events $\xi_j = (w_j, \mu_j, \sigma_j^2)$, $j = 1, \dots, k$, in a region $A \subset \mathbb{R}^3$. Given a reference point $v \in A$, in the same space as the events ξ_j (e.g. $v = (\omega, \mu, \sigma^2)$), then the point-to-nearest-event distance, y , is the distance from the point (v) to the nearest event (ξ_j) in A with respect to some distance measure. One can evaluate distributional aspects of the events

$\{\xi_j\}$, through y , as observed from different reference points v . A diagnostic can then be constructed based on comparisons between empirical distribution functions of the distances y , constructed from Markov chain sample paths. Intuitively, as the Markov chains converge, the distribution functions for y constructed from replicate chains should be similar.

This approach permits the direct comparison of full parameter vectors of varying dimension and, as a result, naturally incorporates a measure of across-model convergence. Due to the manner of their construction, Sisson and Fan (2007) are able to monitor an arbitrarily large number of such diagnostics. However, while this approach may have some appeal, it is limited by the need to construct the model in the marked point process setting. Common models which may be formulated in this framework include finite-mixture, change-point and regression models.

Example: Convergence Assessment for Finite Mixture Univariate Normals

We consider the reversible jump sampler of Richardson and Green (1997) implementing a finite mixture of normals model (Equation 3.5) using the enzymatic activity data set (Figure 3.1b). For the purpose of assessing performance of the sampler, we implement five independent sampler replications of length 400,000 iterations.

Figure 3.2a,b illustrates the diagnostic of Brooks et al. (2003b) which provides a test for between-chain convergence based on posterior model probabilities. The pairwise Kolmogorov–Smirnov and χ^2 (all chains simultaneously) tests assume independent realizations. Based on the estimated convergence rate (Brooks et al., 2003b), we retain every 400th iteration to obtain approximate independence. The Kolmogorov–Smirnov statistic cannot reject immediate convergence, with all pairwise chain comparisons well above the critical value of 0.05. The χ^2 statistic cannot reject convergence after the first 10,000 iterations.

Figure 3.2c illustrates the two multivariate PSRFs of Castelloe and Zimmerman (2002) using the deviance as the default statistic to monitor. The solid line shows the ratio of between- and within-chain variation; the broken line indicates the ratio of within-model variation, and the within-model, within-chain variation. The mPSRFs rapidly approach 1, suggesting convergence, beyond 166,000 iterations. This is supported by the independent analysis of Brooks and Giudici (2000) who demonstrate evidence for convergence of this sampler after around 150,000 iterations, although they caution that their chain lengths of only 200,000 iterations were too short for certainty.

Figure 3.2d, adapted from Sisson and Fan (2007), illustrates the PSRF of the distances from each of 100 randomly chosen reference points to the nearest model components, over the five replicate chains. Up to around 100,000 iterations, between-chain variation is still reducing; beyond 300,000 iterations, differences between the chains appear to have stabilized. The intervening iterations mark a gradual transition between these two states. This diagnostic appears to be the most conservative of those presented here.

This example highlights that empirical convergence assessment tools often give varying estimates of when convergence may have been achieved. As a result, it may be prudent to follow the most conservative estimates in practice. While it is undeniable that the benefits for the practitioner in implementing reversible jump sampling schemes are immense, it is arguable that the practical importance of ensuring chain convergence is often overlooked. However, it is also likely that current diagnostic methods are insufficiently advanced to permit a more rigorous default assessment of sampler convergence.

3.3.3 Estimating Bayes Factors

One of the useful by-products of the reversible jump sampler is the ease with which Bayes factors can be estimated. Explicitly expressing marginal or predictive densities of \mathbf{x} under

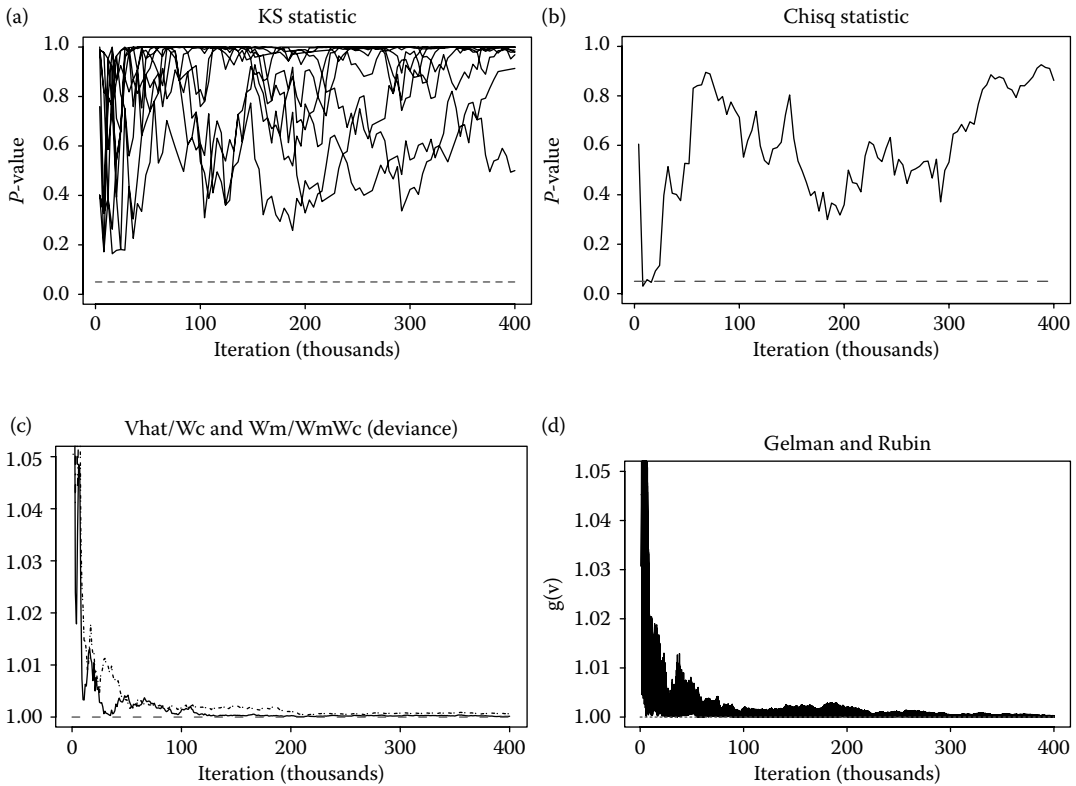


FIGURE 3.2

Convergence assessment for the enzymatic activity data set. (a) Kolmogorov–Smirnov and (b) χ^2 tests of Brooks et al. (2003b). Horizontal line denotes an $\alpha = 0.05$ significance level for test of different sampling distributions. (c) Multivariate PSRFs of Castelloe and Zimmerman (2002) and (d) PSRFVs of Sisson and Fan (2007). Horizontal lines denote the value of each statistic under equal sampling distributions. (From Sisson, S. A. and Fan, Y. 2007. *Statistics and Computing*, 17:357–367. With permission.)

model \mathcal{M}_k as

$$m_k(\mathbf{x}) = \int_{\mathbb{R}^{n_k}} L(\mathbf{x} | k, \boldsymbol{\theta}_k) p(\boldsymbol{\theta}_k | k) d\boldsymbol{\theta}_k,$$

the normalized posterior probability of model \mathcal{M}_k is given by

$$p(k | \mathbf{x}) = \frac{p(k)m_k(\mathbf{x})}{\sum_{k' \in \mathcal{K}} p(k')m_{k'}(\mathbf{x})} = \left(1 + \sum_{k' \neq k} \frac{p(k')}{p(k)} B_{k',k} \right)^{-1},$$

where $B_{k',k} = m_{k'}(\mathbf{x})/m_k(\mathbf{x})$ is the Bayes factor of model $\mathcal{M}_{k'}$ to \mathcal{M}_k , and $p(k)$ is the prior probability of model \mathcal{M}_k . For a discussion of Bayesian model selection techniques, see Chipman et al. (2001), Berger and Pericchi (2001), Kass and Raftery (1995), Ghosh and Samanta (2001), Berger and Pericchi (2004), and Barbieri and Berger (2004). The usual estimator of the posterior model probability, $p(k | \mathbf{x})$, is given by the proportion of chain iterations the reversible jump sampler spent in model \mathcal{M}_k .

However, when the number of candidate models $|\mathcal{M}|$ is large, the use of reversible jump MCMC algorithms to evaluate Bayes factors raises issues of efficiency. Suppose that model

\mathcal{M}_k accounts for a large proportion of posterior mass. In attempting a between-model move from model \mathcal{M}_k , the reversible jump algorithm will tend to persist in this model and visit others models rarely. Consequently, estimates of Bayes factors based on model-visit proportions will tend to be inefficient (Bartolucci and Scaccia, 2003; Han and Carlin, 2001).

Bartolucci et al. (2006) propose enlarging the parameter space of the models under comparison with the same auxiliary variables, $\mathbf{u} \sim q_{d_{k \rightarrow k'}}(\mathbf{u})$ and $\mathbf{u}' \sim q_{d_{k' \rightarrow k}}(\mathbf{u}')$ (see Equation 3.9), defined under the between-model transitions, so that the enlarged spaces, $(\boldsymbol{\theta}_k, \mathbf{u})$ and $(\boldsymbol{\theta}_{k'}, \mathbf{u}')$, have the same dimension. In this setting, an extension to the bridge estimator for the estimation of the ratio of normalizing constants of two distributions (Meng and Wong, 1996) can be used, by integrating out the auxiliary random process (i.e. \mathbf{u} and \mathbf{u}') involved in the between-model moves. Accordingly, the Bayes factor of model $\mathcal{M}_{k'}$ to \mathcal{M}_k can be estimated using the reversible jump acceptance probabilities as

$$\hat{B}_{k',k} = \frac{\sum_{j=1}^{J_k} \alpha^{(j)}[(k, \boldsymbol{\theta}_k), (k', \boldsymbol{\theta}'_{k'})]/J_k}{\sum_{j=1}^{J_{k'}} \alpha^{(j)}[(k', \boldsymbol{\theta}'_{k'}), (k, \boldsymbol{\theta}_k)]/J_{k'}}$$

where $\alpha^{(j)}[(k, \boldsymbol{\theta}_k), (k', \boldsymbol{\theta}'_{k'})]$ is the acceptance probability (Equation 3.9) of the j th attempt to move from model \mathcal{M}_k to $\mathcal{M}_{k'}$, and where J_k and $J_{k'}$ are the number of proposed moves from model \mathcal{M}_k to $\mathcal{M}_{k'}$ and vice versa during the simulation. Further manipulation is required to estimate $B_{k',k}$ if the sampler does not jump between models \mathcal{M}_k and $\mathcal{M}_{k'}$ directly (Bartolucci et al., 2006). This approach can provide a more efficient way of postprocessing reversible jump MCMC with minimal computational effort.

3.4 Related Multi-Model Sampling Methods

Several alternative multi-model sampling methods are available. Some of these are closely related to the reversible jump MCMC algorithm, or include reversible jump as a special case.

3.4.1 Jump Diffusion

Before the development of the reversible jump sampler, Grenander and Miller (1994) proposed a sampling strategy based on continuous-time jump-diffusion dynamics. This process combines jumps between models at random times, and within-model updates based on a diffusion process according to a Langevin stochastic differential equation indexed by time, t , satisfying

$$d\boldsymbol{\theta}_k^t = dB_k^t + \frac{1}{2} \nabla \log \pi(\boldsymbol{\theta}_k^t) dt.$$

where dB_k^t denotes an increment of Brownian motion and ∇ the vector of partial derivatives. This method has found some application in signal processing and other Bayesian analyses (Miller et al., 1995; Phillips and Smith, 1996), but has in general been superseded by the more accessible reversible jump sampler. In practice, the continuous-time diffusion must be approximated by a discrete-time simulation. If the time discretization is corrected for via a Metropolis–Hastings acceptance probability, the jump-diffusion sampler actually results in an implementation of reversible jump MCMC (Besag, 1994).

3.4.2 Product Space Formulations

As an alternative to samplers designed for implementation on unions of model spaces, $\Theta = \bigcup_{k \in \mathcal{K}} (\{k\}, \mathbb{R}^{n_k})$, a number of “supermodel” product-space frameworks have been developed, with a state space given by $\Theta^* = \otimes_{k \in \mathcal{K}} (\{k\}, \mathbb{R}^{n_k})$. This setting encompasses all model spaces jointly, so that a sampler needs to simultaneously track θ_k for all $k \in \mathcal{K}$. The composite parameter vector, $\theta^* \in \Theta^*$, consisting of a concatenation of all parameters under all models, is of fixed dimension, thereby circumventing the necessity of between-model transitions. Clearly, product-space samplers are limited to situations where the dimension of θ^* is computationally feasible. Carlin and Chib (1995) propose a posterior distribution for the composite model parameter and model indicator given by

$$\pi(k, \theta^* | \mathbf{x}) \propto L(\mathbf{x} | k, \theta_{\mathcal{I}_k}^*) p(\theta_{\mathcal{I}_k}^* | k) p(\theta_{\mathcal{I}_{-k}}^* | \theta_{\mathcal{I}_k}^*, k) p(k),$$

where \mathcal{I}_k and \mathcal{I}_{-k} are index sets respectively identifying and excluding the parameters θ_k from θ^* . Here $\mathcal{I}_k \cap \mathcal{I}_{k'} = \emptyset$ for all $k \neq k'$, so that the parameters for each model are distinct. It is easy to see that the term $p(\theta_{\mathcal{I}_{-k}}^* | \theta_{\mathcal{I}_k}^*, k)$, called a “pseudo-prior” by Carlin and Chib (1995), has no effect on the joint posterior $\pi(k, \theta_{\mathcal{I}_k}^* | \mathbf{x}) = \pi(k, \theta_k | \mathbf{x})$, and its form is usually chosen for convenience. However, poor choices may affect the efficiency of the sampler (Godsill, 2003; Green, 2003).

Godsill (2001) proposes a further generalization of the above by relaxing the restriction that $\mathcal{I}_k \cap \mathcal{I}_{k'} = \emptyset$ for all $k \neq k'$. That is, individual model parameter vectors are permitted to overlap arbitrarily, which is intuitive for, say, nested models. This framework can be shown to encompass the reversible jump algorithm, in addition to the setting of Carlin and Chib (1995). In theory this allows for direct comparison between the three samplers, although this has not yet been fully examined. However, one clear point is that the information contained within $\theta_{\mathcal{I}_{-k}}^*$ would be useful in generating efficient between-model transitions when in model \mathcal{M}_k , under a reversible jump sampler. This idea is exploited by Brooks et al. (2003c).

3.4.3 Point Process Formulations

A different perspective on the multi-model sampler is based on spatial birth-and-death processes (Preston, 1977; Ripley, 1977). Stephens (2000a) observed that particular multi-model statistical problems can be represented as continuous-time, marked point processes (Geyer and Møller, 1994). One obvious setting is finite-mixture modeling (Equation 3.5) where the birth and death of mixture components, ϕ_j , indicate transitions between models. The sampler of Stephens (2000a) may be interpreted as a particular continuous-time, limiting version of a sequence of reversible jump algorithms (Cappé et al., 2003).

A number of illustrative comparisons of the reversible jump, jump diffusion, product space and point process frameworks can be found in the literature. See, for example, Andrieu et al. (2001), Dellaportas et al. (2002), Carlin and Chib (1995), Godsill (2001, 2003), Cappé et al. (2003), and Stephens (2000a).

3.4.4 Multi-Model Optimization

The reversible jump MCMC sampler may be utilized as the underlying random mechanism within a stochastic optimization framework, given its ability to traverse complex spaces efficiently (Andrieu et al., 2000; Brooks et al., 2003a). In a simulated annealing setting, the

sampler would define a stationary distribution proportional to the Boltzmann distribution

$$B_T(k, \theta_k) \propto \exp \left\{ \frac{-f(k, \theta_k)}{T} \right\},$$

where $T \geq 0$ and $f(k, \theta_k)$ is a model-ranking function to be minimized. A stochastic annealing framework will then decrease the value of T according to some schedule while using the reversible jump sampler to explore function space. Assuming adequate chain mixing, as $T \rightarrow 0$ the sampler and the Boltzmann distribution will converge to a point mass at $(k^*, \theta_{k^*}^*) = \arg \max f(k, \theta_k)$. Specifications for the model-ranking function may include the Akaike information criterion or Bayesian information criterion (King and Brooks, 2004; Sisson and Fan, 2009), the posterior model probability (Clyde, 1999) or a nonstandard loss function defined on variable-dimensional space (Sisson and Hurn, 2004) for the derivation of Bayes rules.

3.4.5 Population MCMC

The population Markov chain Monte Carlo method (Liang and Wong, 2001; Liu, 2001) may be extended to the reversible jump setting (Jasra et al., 2007). Motivated by simulated annealing (Geyer and Thompson, 1995), N parallel reversible jump samplers are implemented targeting a sequence of related distributions $\{\pi_i, i = 1, \dots, N$, which may be tempered versions of the distribution of interest, $\pi_1 = \pi(k, \theta_k | \mathbf{x})$. The chains are allowed to interact, in that the states of any two neighboring (in terms of the tempering parameter) chains may be exchanged, thereby improving the mixing across the population of samplers both within and between models. Jasra et al. (2007) demonstrate superior convergence rates over a single reversible jump sampler. For samplers that make use of tempering or parallel simulation techniques, Gramacy et al. (2010) propose efficient methods of utilizing samples from all distributions (i.e. including those not from π_1) using importance weights, for the calculation of given estimators.

3.4.6 Multi-Model Sequential Monte Carlo

The idea of running multiple samplers over a sequence of related distributions may also be considered under a sequential Monte Carlo (SMC) framework (Del Moral et al., 2006). Jasra et al. (2008) propose implementing N separate SMC samplers, each targeting a different subset of model space. At some stage the samplers are allowed to interact and are combined into a single sampler. This approach permits more accurate exploration of models with lower posterior model probabilities than would be possible under a single sampler. As with population MCMC methods, the benefits gained in implementing N samplers must be weighed against the extra computational overheads.

3.5 Discussion and Future Directions

Given the degree of complexity associated with the implementation of reversible jump MCMC, a major focus for future research is in designing simple but efficient samplers, with the ultimate goal of automation. Several authors have provided new insights into the

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reversible jump sampler which may contribute toward achieving such goals. For example, Keith et al. (2004) present a generalized Markov sampler, which includes the reversible jump sampler as a special case. Petris and Tardella (2003) demonstrate a geometric approach for sampling from nested models, formulated by drawing from a fixed-dimension auxiliary continuous distribution on the largest model subspace, and then using transformations to recover model-specific samples. Walker (2009) has recently provided a Gibbs sampler alternative to the reversible jump MCMC, using auxiliary variables. Additionally, as noted by Sisson (2005), one does not need to work only with reversible Markov chains, and nonreversible chains may offer opportunities for sampler improvement (Diaconis et al., 2000; Mira and Geyer, 2000; Neal, 2004).

An alternative way of increasing sampler efficiency would be to explore the ideas introduced in adaptive MCMC. As with standard MCMC, any adaptations must be implemented with care—transition kernels dependent on the entire history of the Markov chain can only be used under diminishing adaptation conditions (Haario et al., 2001; Roberts and Rosenthal, 2009). Alternative schemes permit modification of the proposal distribution at regeneration times, when the next state of the Markov chain becomes completely independent of the past (Brockwell and Kadane, 2005; Gilks et al., 1998). Under the reversible jump framework, regeneration can be naturally achieved by incorporating an additional model, from which independent samples can be drawn. Under any adaptive scheme, however, how best to make use of historical chain information remains an open question. Additionally, efficiency gains through adaptations should naturally outweigh the costs of handling chain history and modification of the proposal mechanisms.

Finally, two areas remain underdeveloped in the context of reversible jump simulation. The first of these is perfect simulation, which provides an MCMC framework for producing samples exactly from the target distribution, circumventing convergence issues entirely (Propp and Wilson, 1996). Some tentative steps have been made in this area (Brooks et al., 2006; Møller and Nicholls, 1999). Secondly, while the development of “likelihood-free” MCMC has received much recent attention (Chapter 12, this volume), implementing the sampler in the multi-model setting remains a challenging problem, in terms of both computational efficiency and bias of posterior model probabilities.

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References

- Al-Awadhi, F., Hurn, M. A., and Jennison, C. 2004. Improving the acceptance rate of reversible jump MCMC proposals. *Statistics and Probability Letters*, 69:189–198.
- Andrieu, C., de Freitas, J., and Doucet, A. 2000. Reversible jump MCMC simulated annealing for neural networks. In C. Boutilier and M. Goldszmidt (eds), *Proceedings of the 16th Conference on Uncertainty in Artificial Intelligence*, pp. 11–18. Morgan Kaufmann, San Francisco.
- Andrieu, C., Djurić, P. M., and Doucet, M. 2001. Model selection by MCMC computation. *Signal Processing*, 81:19–37.

- Barbieri, M. M. and Berger, J. O. 2004. Optimal predictive model selection. *Annals of Statistics*, 32:870–897.
- Bartolucci, F. and Scaccia, L. 2003. A new approach for estimating the Bayes factor. Technical report, University of Perugia.
- Bartolucci, F., Scaccia, L., and Mira, A. 2006. Efficient Bayes factors estimation from reversible jump output. *Biometrika*, 93(1):41–52.
- Berger, J. O. and Pericchi, L. R. 2001. Objective Bayesian methods for model selection: Introduction and comparison (with discussion). In P. Lahiri (ed.), *Model Selection*, IMS Lecture Notes—Monograph Series, 38, pp. 135–207. Institute of Mathematical Statistics, Beachwood, OH.
- Berger, J. O. and Pericchi, L. R. 2004. Training samples in objective Bayesian model selection. *Annals of Statistics*, 32:841–869.
- Besag, J. 1994. Contribution to the discussion of a paper by Grenander and Miller. *Journal of the Royal Statistical Society, Series B*, 56:591–592.
- Brockwell, A. E. and Kadane, J. B. 2005. Identification of regeneration times in MCMC simulation, with application to adaptive schemes. *Journal of Computational and Graphical Statistics*, 14(2): 436–458.
- Brooks, S. P. 1998. Markov chain Monte Carlo method and its application. *The Statistician*, 47: 69–100.
- Brooks, S. P. and Giudici, P. 2000. MCMC convergence assessment via two-way ANOVA. *Journal of Computational and Graphical Statistics*, 9:266–285.
- Brooks, S. P., Fan, Y., and Rosenthal, J. S. 2006. Perfect forward simulation via simulated tempering. *Communications in Statistics*, 35:683–713.
- Brooks, S. P., Friel, N., and King, R. 2003a. Classical model selection via simulated annealing. *Journal of the Royal Statistical Society, Series B*, 65:503–520.
- Brooks, S. P., Giudici, P., and Philippe, A. 2003b. On non-parametric convergence assessment for MCMC model selection. *Journal of Computational and Graphical Statistics*, 12:1–22.
- Brooks, S. P., Giudici, P., and Roberts, G. O. 2003c. Efficient construction of reversible jump Markov chain Monte Carlo proposal distributions (with discussion). *Journal of the Royal Statistical Society, Series B*, 65:3–39.
- Cappé, O., Robert, C. P., and Rydén, T. 2003. Reversible jump MCMC converging to birth-and-death MCMC and more general continuous time samplers. *Journal of the Royal Statistical Society, Series B*, 65:679–700.
- Carlin, B. P. and Chib, S. 1995. Bayesian model choice via Markov chain Monte Carlo. *Journal of the Royal Statistical Society, Series B*, 57:473–484.
- Castelloe, J. M. and Zimmerman, D. L. 2002. Convergence assessment for reversible jump MCMC samplers. Technical Report 313, Department of Statistics and Actuarial Science, University of Iowa.
- Celeux, G., Hurn, M. A., and Robert, C. P. 2000. Computational and inferential difficulties with mixture posterior distributions. *Journal of the American Statistical Association*, 95:957–970.
- Chipman, H., George, E., and McCulloch, R. E. 2001. The practical implementation of Bayesian model selection (with discussion). In P. Lahiri (ed.), *Model Selection*, IMS Lecture Notes—Monograph Series, 38, pp. 67–134. Institute of Mathematical Statistics, Beachwood, OH.
- Clyde, M. A. 1999. Bayesian model averaging and model search strategies. In J. M. Bernardo, J. O. Berger, A. P. Dawid, and A. F. M. Smith (eds), *Bayesian Statistics 6: Proceedings of the Sixth Valencia International Meeting*, pp. 157–185. Oxford University Press, Oxford.
- Cowles, M. K. and Carlin, B. P. 1996. Markov chain Monte Carlo convergence diagnostics: A comparative review. *Journal of the American Statistical Association*, 91:883–904.
- Del Moral, P., Doucet, A., and Jasra, A. 2006. Sequential Monte Carlo samplers. *Journal of the Royal Statistical Society, Series B*, 68:411–436.
- Dellaportas, P. and Papageorgiou, I. 2006. Multivariate mixtures of normals with unknown number of components. *Statistics and Computing*, 16:57–68.
- Dellaportas, P., Forster, J. J., and Ntzoufras, I. 2002. On Bayesian model and variable selection using MCMC. *Statistics and Computing*, 12:27–36.

- Denison, D. G. T., Mallick, B. K., and Smith, A. F. M. 1998. Automatic Bayesian curve fitting. *Journal of the Royal Statistical Society, Series B*, 60:330–350.
- Diaconis, P., Holmes, S., and Neal, R. M. 2000. Analysis of a non-reversible Markov chain sampler. *Annals of Applied Probability*, 10:726–752.
- Diggle, P. J. 1983. *Statistical Analysis of Spatial Point Patterns*. Academic Press, London.
- DiMatteo, I., Genovese, C. R., and Kass, R. E. 2001. Bayesian curve-fitting with free-knot splines. *Biometrika*, 88:1055–1071.
- Ehlers, R. S. and Brooks, S. P. 2003. Constructing general efficient proposals for reversible jump MCMC. Technical report, Department of Statistics, Federal University of Paraná.
- Ehlers, R. S. and Brooks, S. P. 2008. Adaptive proposal construction for reversible jump MCMC. *Scandinavian Journal of Statistics*, 35:677–690.
- Fan, Y. and Brooks, S. P. 2000. Bayesian modelling of prehistoric corbelled domes. *The Statistician*, 49:339–354.
- Fan, Y., Peters, G. W., and Sisson, S. A. 2009. Automating and evaluating reversible jump MCMC proposal distributions. *Statistics and Computing*, 19(4):409–421.
- Frühwirth-Schnatter, S. 2001. Markov chain Monte Carlo estimation of classical and dynamic switching and mixture models. *Journal of the American Statistical Association*, 96:194–209.
- Gelman, A. and Rubin, D. B. 1992. Inference from iterative simulations using multiple sequences. *Statistical Science*, 7:457–511.
- George, A. W., Mengersen, K. L., and Davis, G. P. 1999. A Bayesian approach to ordering gene markers. *Biometrics*, 55:419–429.
- George, E. I. and McCulloch, R. E. 1993. Variable selection via Gibbs sampling. *Journal of the American Statistical Association*, 88:881–889.
- Geyer, C. J. and Möller, J. 1994. Simulation procedures and likelihood inference for spatial point processes. *Scandinavian Journal of Statistics*, 21:359–373.
- Geyer, C. J. and Thompson, E. A. 1995. Annealing Markov chain Monte Carlo with applications to ancestral inference. *Journal of the American Statistical Association*, 90:909–920.
- Ghosh, J. K. and Samanta, T. 2001. Model selection: An overview. *Current Science*, 80:1135–1144.
- Gilks, W. R., Roberts, G. O., and Sahu, S. K. 1998. Adaptive Markov chain Monte Carlo through regeneration. *Journal of the American Statistical Association*, 93:1045–1054.
- Godsill, S. 2001. On the relationship between Markov chain Monte Carlo methods for model uncertainty. *Journal of Computational and Graphical Statistics*, 10:1–19.
- Godsill, S. 2003. Discussion of Trans-dimensional Markov chain Monte Carlo by P. J. Green. In P. J. Green, N. L. Hjort, and S. Richardson (eds), *Highly Structured Stochastic Systems*, pp. 199–203. Oxford University Press, Oxford.
- Gramacy, R. B., Samworth, R. J., and King, R. 2010. Importance tempering. *Statistics and Computing*, 20:1–7.
- Green, P. J. 1995. Reversible jump Markov chain Monte Carlo computation and Bayesian model determination. *Biometrika*, 82:711–732.
- Green, P. J. 2001. A primer on Markov chain Monte Carlo. In O. E. Barndorff-Nielsen, D. R. Cox, and C. Klüppelberg (eds), *Complex Stochastic Systems*, Monographs on Statistics and Probability, 87, pp. 1–62. Chapman & Hall/CRC, Boca Raton, FL.
- Green, P. J. 2003. Trans-dimensional Markov chain Monte Carlo. In P. J. Green, N. L. Hjort, and S. Richardson (eds), *Highly Structured Stochastic Systems*, pp. 179–198. Oxford University Press, Oxford.
- Green, P. J. and Mira, A. 2001. Delayed rejection in reversible jump Metropolis-Hastings. *Biometrika*, 88:1035–1053.
- Grenander, U. and Miller, M. I. 1994. Representations of knowledge in complex systems. *Journal of the Royal Statistical Society, Series B*, 56:549–603.
- Haario, H., Saksman, E., and Tamminen, J. 2001. An adaptive Metropolis algorithm. *Bernoulli*, 7: 223–242.
- Han, C. and Carlin, B. P. 2001. MCMC methods for computing Bayes factors: A comparative review. *Journal of the American Statistical Association*, 96:1122–1132.

- Hastie, D. 2004. Developments in Markov chain Monte Carlo. PhD thesis, University of Bristol.
- Hastie, T. J. and Tibshirani, R. J. 1990. *Generalised Additive Models*. Chapman & Hall, London.
- Hastings, W. K. 1970. Monte Carlo sampling methods using Markov chains and their applications. *Biometrika*, 57:59–109.
- Hurn, M., Justel, A., and Robert, C. P. 2003. Estimating mixtures of regressions. *Journal of Computational and Graphical Statistics*, 12:55–79.
- Jasra, A., Doucet, A., Stephens, D. A., and Holmes, C. 2008. Interacting sequential Monte Carlo samplers for trans-dimensional simulation. *Computational Statistics and Data Analysis*, 52(4): 1765–1791.
- Jasra, A., Holmes, C., and Stephens, D. A. 2005. MCMC methods and the label switching problem. *Statistical Science*, 20(1):50–67.
- Jasra, A., Stephens, D. A., and Holmes, C. C. 2007. Population-based reversible jump Markov chain Monte Carlo. *Biometrika*, 94:787–807.
- Kass, R. E. and Raftery, A. E. 1995. Bayes factors. *Journal of the American Statistical Association*, 90:773–796.
- Keith, J. M., Kroese, D. P., and Bryant, D. 2004. A generalized Markov sampler. *Methodology and Computing in Applied Probability*, 6:29–53.
- King, R. and Brooks, S. P. 2004. A classical study of catch-effort models for Hector's dolphins. *Journal of the American Statistical Association*, 99:325–333.
- Kirkpatrick, S. 1984. Optimization by simulated annealing: Quantitative studies. *Journal of Statistical Physics*, 34:975–986.
- Lawler, G. and Sokal, A. 1988. Bounds on the L^2 spectrum for Markov chains and Markov processes. *Transactions of the American Mathematical Society*, 309:557–580.
- Liang, F. and Wong, W. H. 2001. Real parameter evolutionary Monte Carlo with applications to Bayesian mixture models. *Journal of the American Statistical Association*, 96:653–666.
- Liu, J. S. 2001. *Monte Carlo Strategies in Scientific Computing*. Springer, New York.
- Liu, J. S., Liang, F., and Wong, W. H. 2001. A theory for dynamic weighing in Monte Carlo computation. *Journal of the American Statistical Association*, 96(454):561–573.
- Meng, X. L. and Wong, W. H. 1996. Simulating ratios of normalising constants via a simple identity: A theoretical exploration. *Statistica Sinica*, 6:831–860.
- Mengersen, K. L., Robert, C. P., and Guihenneuc-Joyaux, C. 1999. MCMC convergence diagnostics: A review. In J. M. Bernardo, J. O. Berger, A. P. Dawid, and A. F. M. Smith (eds), *Bayesian Statistics 6*, pp. 415–140. Oxford University Press, Oxford.
- Miller, M. I., Srivastava, A., and Grenander, U. 1995. Conditional-mean estimation via jump-diffusion processes in multiple target tracking/recognition. *IEEE Transactions on Signal Processing*, 43:2678–2690.
- Mira, A. and Geyer, C. J. 2000. On non-reversible Markov chains. In N. Madras (ed.), *Monte Carlo Methods*, pp. 93–108. American Mathematical Society, Providence, RI.
- Møller, J. and Nicholls, G. K. 1999. Perfect simulation for sample-based inference. Technical report, Aalborg University.
- Neal, R. M. 2004. Improving asymptotic variance of MCMC estimators: Non-reversible chains are better. Technical Report 0406, Department of Statistics, University of Toronto.
- Nott, D. J. and Green, P. J. 2004. Bayesian variable selection and the Swendsen-Wang algorithm. *Journal of Computational and Graphical Statistics*, 13(1):141–157.
- Nott, D. J. and Leonte, D. 2004. Sampling schemes for Bayesian variable selection in generalised linear models. *Journal of Computational and Graphical Statistics*, 13(2):362–382.
- Ntzoufras, I., Dellaportas, P., and Forster, J. J. 2003. Bayesian variable and link determination for generalised linear models. *Journal of Statistical Planning and Inference*, 111:165–180.
- Papathomas, M., Dellaportas, P., and Vasdekis, V. G. S. 2009. A general proposal construction for reversible jump MCMC. Technical report, Athens University of Economics and Business.
- Peskun, P. 1973. Optimum Monte Carlo sampling using Markov chains. *Biometrika*, 60:607–612.

- Petris, G. and Tardella, L. 2003. A geometric approach to transdimensional Markov chain Monte Carlo. *Canadian Journal of Statistics*, 31.
- Phillips, D. B. and Smith, A. F. M. 1996. Bayesian model comparison via jump diffusions. In W. R. Gilks, S. Richardson, and D. J. Spiegelhalter (eds), *Markov Chain Monte Carlo in Practice*, pp. 215–239. Chapman & Hall, London.
- Preston, C. J. 1977. Spatial birth-and-death processes. *Bulletin of the International Statistical Institute*, 46:371–391.
- Propp, J. G. and Wilson, D. B. 1996. Exact sampling with coupled Markov chains and applications to statistical mechanics. *Random Structures and Algorithms*, 9:223–252.
- Richardson, S. and Green, P. J. 1997. On Bayesian analysis of mixtures with an unknown number of components (with discussion). *Journal of the Royal Statistical Society, Series B*, 59: 731–792.
- Ripley, B. D. 1977. Modelling spatial patterns (with discussion). *Journal of the Royal Statistical Society, Series B*, 39:172–212.
- Roberts, G. O. 2003. Linking theory and practice of MCMC. In P. J. Green, N. Hjort, and S. Richardson (eds), *Highly Structured Stochastic Systems*, pp. 145–166. Oxford University Press.
- Roberts, G. O. and Rosenthal, J. S. 2009. Examples of adaptive MCMC. *Journal of Computational and Graphical Statistics*, 18:349–367.
- Sisson, S. A. 2005. Trans-dimensional Markov chains: A decade of progress and future perspectives. *Journal of the American Statistical Association*, 100:1077–1089.
- Sisson, S. A. and Fan, Y. 2007. A distance-based diagnostic for trans-dimensional Markov chains. *Statistics and Computing*, 17:357–367.
- Sisson, S. A. and Fan, Y. 2009. Towards automating model selection for a mark-recapture-recovery analysis. *Applied Statistics*, 58(2):247–266.
- Sisson, S. A. and Hurn, M. A. 2004. Bayesian point estimation of quantitative trait loci. *Biometrics*, 60:60–68.
- Smith, M. and Kohn, R. 1996. Nonparametric regression using Bayesian variable selection. *Journal of Econometrics*, 75:317–344.
- Stephens, M. 2000a. Bayesian analysis of mixture models with an unknown number of components—an alternative to reversible jump methods. *Annals of Statistics*, 28:40–74.
- Stephens, M. 2000b. Dealing with label switching in mixture models. *Journal of the Royal Statistical Society, Series B*, 62:795–809.
- Tadesse, M., Sha, N., and Vannucci, M. 2005. Bayesian variable selection in clustering high-dimensional data. *Journal of the American Statistical Association*, 100:602–617.
- Tierney, L. 1998. A note on Metropolis–Hastings kernels for general state spaces. *Annals of Applied Probability*, 8:1–9.
- Tierney, L. and Mira, A. 1999. Some adaptive Monte Carlo methods for Bayesian inference. *Statistics in Medicine*, 18:2507–2515.
- Trias, M., Vecchio, A., and Vetch, J. 2009. Delayed rejection schemes for efficient Markov chain Monte Carlo sampling of multimodal distributions. Technical report, Universitat de les Illes Balears.
- Vermaak, J., Andrieu, C., Doucet, A., and Godsill, S. J. 2004. Reversible jump Markov chain Monte Carlo strategies for Bayesian model selection in autoregressive processes. *Journal of Time Series Analysis*, 25(6):785–809.
- Walker, S. G. 2009. A Gibbs sampling alternative to reversible jump MCMC. Technical report, University of Kent.